Precursors of Antiferromagnetic and Hubbard Bands in the 2D Hubbard Model

Bumsoo Kyung
Max Planck Institute for Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany
(5 December 1997)

We formulate a theory to the 2D Hubbard model in a framework free of finite size effect and numerical analytical continuation, yet containing the essential features of the 2D Hubbard model, i.e., the correct atomic limit for large frequencies and 2D spin fluctuations. As temperature is decreased for a 2D half-filled band, 2D critical fluctuations give rise to a strong local maximum in $\mid Im\Sigma(\vec{k}_F,\omega) \mid$ at $\omega = 0$ leading to a split peak in the spectral function. As U is increased, four peaks associated with antiferromagnetic and Hubbard bands begin to develop in small and intermediate frequency regimes.

PACS numbers: 71.10.Fd, 71.27.+a

Recently the Hubbard model has received considerable attention, since it is believed to contain the essential physics of strong electron correlations found in the high temperature superconductors [1]. Although it was solved exactly in one-dimension [2], the exact solution in higher dimensions is not known yet. For a half-filled 2D band, the $T = 0$ ground state is believed to be antiferromagnetic insulating for all U, while at finite temperatures strong spin fluctuations destroy long-range antiferromagnetic order due to the Mermin-Wagner theorem [3].

In the absence of a small expansion parameter of the model in the physically relevant regime, quantum Monte Carlo (QMC) simulations have played an important role in elucidating various dynamical properties at finite temperatures [4]. In spite of its exact nature, QMC calculations suffer from two serious limitations, namely, small lattice size and numerical analytical continuation from imaginary frequencies to real ones. In fact, depending on lattice size and on the method used to extract $A(\vec{k},\omega)$ from $G(\vec{k},i\omega_n)$ computed by QMC, conflicting results have been reported for the single particle spectral function along the antiferromagnetic zone boundary for a half-filled 2D band with $U = 4t$ and $T = 0.1 - 0.25t$ [5,6]. Although calculations based on the lowest order diagram (second order in U) show the correct atomic limit for large ω, they fail to describe the correct 2D spin fluctuations. This atomic limit is reflected as the correct asymptotic behavior of the self-energy at large frequencies, $U^2n/2(1-n/2)/i\omega_n$ (in the paramagnetic state), which is necessary to produce the Hubbard bands at large enough U. Recently fluctuation exchange (FLEX) approximation was applied to the 2D Hubbard model by Bickers *et al.* [7] and later extensively used by Bickers *et al.* [8] and by Dahm *et al.* [9]. Despite its successful application to the D-wave superconductivity and many other issues, it was pointed out by Vilk and Tremblay [10] that FLEX approximation does not show both the precursors of antiferromagnetic and Hubbard bands resulting from the correct 2D spin fluctuations and atomic limit for large ω, respectively. This is because FLEX approximation completely neglects the frequency dependent vertex corrections for the self-energy within its self-consistent structure. While the 2D spin fluctuations were quite successfully described by Vilk and Tremblay [10] by imposing the exact sumrules on the spin and charge susceptibilities, their self-energy does not show the correct asymptotic behavior at large frequencies. Therefore, it is highly desirable to formulate an approximation scheme for the 2D Hubbard model in a manner free of finite size effect and numerical analytical continuation, yet containing the essential features of the 2D Hubbard model, i.e., the correct atomic limit for large ω and 2D spin fluctuations. In this Letter, we propose such a theory for the first time.

We begin with reconsideration of paramagnon theory first proposed by Berk and Schrieffer [11]. This theory has some good features, namely, explicitly enforcing the rotational invariance of the spin susceptibilities together with including the particle-particle channel, and the correct prediction of the zero temperature phase transition for any U in the half-filled 2D band. This theory, however, always gives rise to a finite temperature antiferromagnetic instability for large enough U due to the insufficient treatment of strong 2D spin fluctuations, in conflict with the Mermin-Wagner theorem. At frequencies larger than the bandwidth $W = 8$, the self-energy obtained from this theory is not guaranteed to give the correct asymptotic behavior. Recently we found that within the same structure for the self-energy and various susceptibilities as that in the paramagnon theory, both the Mermin-Wagner theorem and correct atomic limit for large ω can be satisfied simultaneously by introducing renormalized interaction constants U_{sp}, U_{ch}, and U_{pp} in the spin, charge, and particle-particle channels,

respectively.

In our formulation the self-energy is expressed in terms of these renormalized interaction strengths to be determined later:

$$\Sigma(k) = \frac{U^2 T}{N} \sum_q \Bigg\{ \Bigg[\chi^0_{ph}(q) + \frac{3}{2}\chi^0_{ph}(q)\Big(\frac{1}{1 - U_{sp}\chi^0_{ph}(q)} - 1\Big) + \frac{1}{2}\chi^0_{ph}(q)\Big(\frac{1}{1 + U_{ch}\chi^0_{ph}(q)} - 1\Big)\Bigg] G^0(k-q) - \Bigg[\chi^0_{pp}(q)\Big(\frac{1}{1 + U_{pp}\chi^0_{pp}(q)} - 1\Big)\Bigg] G^0(q-k) \Bigg\} . \quad (1)$$

T, N and U are the absolute temperature, number of lattice sites and Coulomb repulsion energy. k is a compact notation for $(\vec{k}, i\omega_n)$ where $i\omega_n$ are either Fermionic or Bosonic Matsubara frequencies. $G^0(k)$ is the noninteracting Green's function and $\chi^0_{ph}(q)$, $\chi^0_{pp}(q)$ are irreducible particle-hole and particle-particle susceptibilities, respectively, which are computed from

$$\chi^0_{ph}(q) = -\frac{T}{N}\sum_k G^0(k-q)G^0(k)$$
$$\chi^0_{pp}(q) = \frac{T}{N}\sum_k G^0(q-k)G^0(k) . \quad (2)$$

Dynamical spin, charge and particle-particle susceptibilities are calculated by

$$\chi_{sp}(q) = \frac{2\chi^0_{ph}(q)}{1 - U_{sp}\chi^0_{ph}(q)}$$
$$\chi_{ch}(q) = \frac{2\chi^0_{ph}(q)}{1 + U_{ch}\chi^0_{ph}(q)}$$
$$\chi_{pp}(q) = \frac{\chi^0_{pp}(q)}{1 + U_{pp}\chi^0_{pp}(q)} . \quad (3)$$

We determine U_{sp}, U_{ch}, and U_{pp} by imposing the following three exact sumrules to Eq. (3):

$$\frac{T}{N}\sum_q \chi_{sp}(q) = n - 2\langle n_\uparrow n_\downarrow\rangle$$
$$\frac{T}{N}\sum_q \chi_{ch}(q) = n + 2\langle n_\uparrow n_\downarrow\rangle - n^2$$
$$\frac{T}{N}\sum_q \chi_{pp}(q) = \langle n_\uparrow n_\downarrow\rangle , \quad (4)$$

where the Pauli exclusion principle $\langle n_\sigma^2\rangle = \langle n_\sigma\rangle$ is explicitly used in the spin and charge channels. By finding U_{sp}, U_{ch} and U_{pp} through Eq. (4), any possible magnetic instability can happen only at zero temperature, because the right hand sides are always finite, in consistency with the Mermin-Wagner theorem. The first two sumrules in Eq. 4 were previously used by Vilk and Tremblay [12] to study collective spin and charge fluctuations in the 2D Hubbard model. The correct asymptotic behavior of the self-energy at large frequencies can be easily checked by substituting Eq. (4) and $\langle n_\uparrow n_\downarrow\rangle = n^2/4$ for noninteracting electrons into Eq. (1). By making an ansatz $U_{sp} \equiv U\langle n_\uparrow n_\downarrow\rangle/(\langle n_\uparrow\rangle\langle n_\downarrow\rangle)$ [12], the double occupancy is computed self-consistently in the first sumrule in Eq. (4) and U_{ch}, U_{pp} can be obtained by the other two sumrules. Throughout the calculations the unit of energy is t. We used a 128×128 lattice in momentum space and performed the calculations by means of well-established fast Fourier transforms (FFT). It should be also noted that we used a real frequency formulation in Eqs. (1)-(4) to avoid any possible uncertainties associated with numerical analytical continuation.

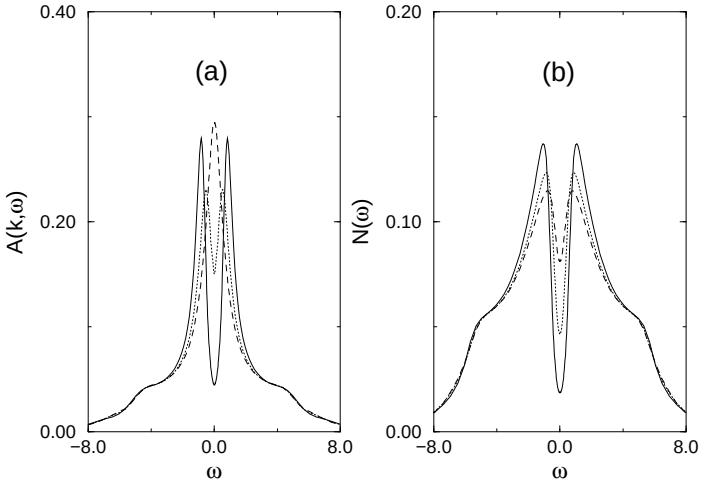

FIG. 1. (a) Spectral functions at $\vec{k} = (\pi/2, \pi/2)$ and (b) density of states, for $U = 4$ at T =0.10, 0.15 and 0.20 denoted as the solid, dotted and dashed curves, respectively.

As a first application of the present theory to the 2D Hubbard model, we study the half-filled 2D Hubbard model in the intermediate coupling regime ($U = 4$) where QMC calculations have shown conflicting results for the single particle spectral function at the noninteracting Fermi surface [5,6]. In this Letter we would like to give a definitive answer to this issue for the first time. The spectral functions at $\vec{k} = (\pi/2, \pi/2)$ and the density of states are presented in Fig. 1(a) and (b) for $U = 4$ at $T = 0.1$, 0.15, and 0.2. At $T = 0.2$ (dashed curve in Fig. 1(a)) a single quasiparticle peak is found at the Fermi energy. As the temperature is slightly decreased to $T = 0.15$ (dotted curve), the single particle peak begins to split into two, leading to a pseudogap [13] at the Fermi energy. This is a precursor of antiferromagnetic bands resulting from strong 2D spin fluctuations at low temperatures. At $T = 0.1$ (solid curve), the two peak structure with a pseudogap inside becomes much more pronounced. The present results support the existence of a pseudogap in the spectral function at $T < 0.2$ for $U = 4$. For all three temperatures, however, the density

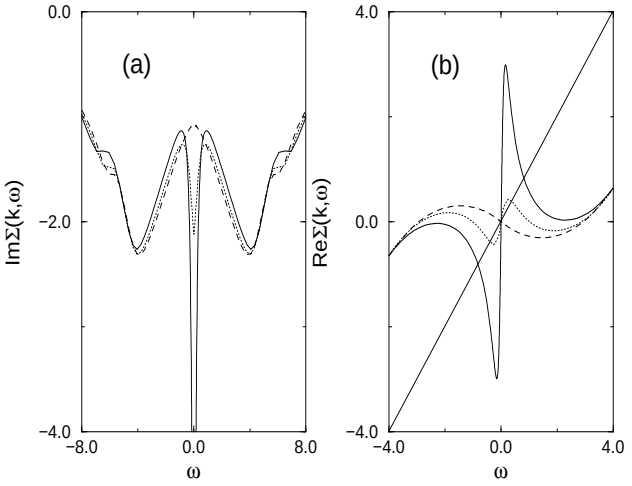

FIG. 2. (a) Imaginary and (b) real parts of the self-energy at $\vec{k} = (\pi/2, \pi/2)$ for $U = 4$ at T =0.1, 0.15 and 0.2 denoted as the solid, dotted and dashed curves, respectively. The solid straight line in (b) is $\omega - \varepsilon(\vec{k})$.

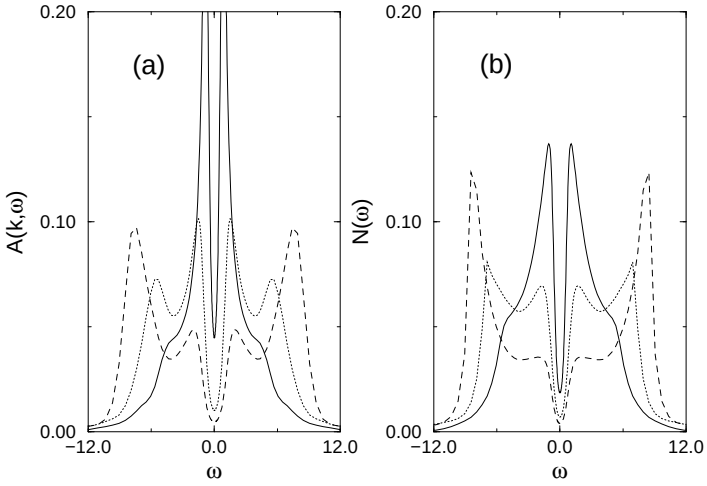

FIG. 3. (a) Spectral functions at $\vec{k} = (\pi/2, \pi/2)$ and (b) density of states, for U =4, 6 and 8 at $T = 0.1$ denoted as the solid, dotted and dashed curves, respectively.

of states (Fig. 1(b)) shows a pseudogap at the Fermi energy. In spite of a single peak structure in the spectral function for $T = 0.2$ (dashed curve), the density of states is significantly suppressed at the Fermi energy compared with that for non-interacting electrons which shows a logarithmic divergence. Because of its accumulative nature, the density of states appears more sensitive to the change of a quasiparticle state at the Fermi energy than the spectral function itself does, at least, for a half-filled 2D band. This situation for $T = 0.2$ is the best result found by Dahm *et al.* [9] within FLEX approximation in an effort to see the precursor effect of the antiferromagnetic bands. The small bumps at $\pm(4-5)t$ both in the spectral function and density of states are precursors of the Hubbard bands, which will be discussed later.

This anomalous behavior is understood more clearly by examining the imaginary and real parts of the self-energy shown in Fig. 2(a) and Fig. 2(b), respectively for the same parameters as in Fig. 1. At $T = 0.2$ (dashed curve), the imaginary part of the self-energy becomes smaller in magnitude as the Fermi energy is approached, indicating a Fermi liquid-like behavior. As the temperature is further decreased to $T = 0.15$ (dotted curve) to $T = 0.1$ (solid curve), however, a drastic change happens near the Fermi energy. Due to 2D critical fluctuations, the scattering rates at the Fermi energy grow exponentially as $\sim \xi \sim exp(constant/T)$. This singular scattering by exchange of strong 2D spin fluctuations is responsible for the strong suppression of the spectral weight at the Fermi energy, leading to the formation of a pseudogap in the spectral function.

The corresponding real part of the self-energy obtained from the imaginary part by means of the Kramers-Kronig relations is shown in Fig. 2(b). The peak condition in the spectral function is determined by the intersection of the real part of the self-energy and $\omega = \varepsilon(\vec{k})$ denoted as the solid straight line in Fig. 2(b). $\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y)$ for nearest neighbor hopping. At $T = 0.2$ (dashed curve), the peak condition is satisfied only at the Fermi energy with its slope being negative, a characteristic feature of the Fermi liquid. As the temperature is decreased to $T = 0.15$ (dotted curve) to $T = 0.1$ (solid curve), its slope becomes positive and larger than unity at the Fermi energy, and thus the peak condition is satisfied at three different locations. Because of large scattering rates at the Fermi energy, however, only two peaks appear in the spectral function, consistent with the results in Fig. 1.

Since the present formulation for the 2D Hubbard model can describe quite reasonably both 2D critical spin fluctuations and the correct atomic limit for large ω, it is of great interest to examine how the precursors of antiferromagnetic and Hubbard bands evolve as the interaction strength is increased. For $U = 4$ (solid curve in Fig. 3(a)), a split peak with developing small bumps at $\pm(4-5)t$ is found. As U is increased to 6 (dashed curve), the antiferromagnetic bands become significantly suppressed and the Hubbard bands grow substantially near ± 6. For $U = 8$ (solid curve), the spectral weight inside the Hubbard bands becomes further suppressed due to the large Coulomb repulsion, and as a result the spectral weight associated with the Hubbard bands becomes dominating over that with the antiferromagnetic bands. The Hubbard bands for $U = 8$ occur at larger frequencies than $\pm U/2$, since the asymptotic behavior of the self-energy, $U^2 n/2(1-n/2)/i\omega_n$, sets in at much higher frequencies than the bandwidth. This is because the strong maximum of the scattering rates at the Fermi energy significantly enhances the real part up to high frequencies. The appearance of four peaks in the spectral function for $U = 8$ is consistent with recent QMC calculations [14,15] except a difference in the relative strength of the two dif-

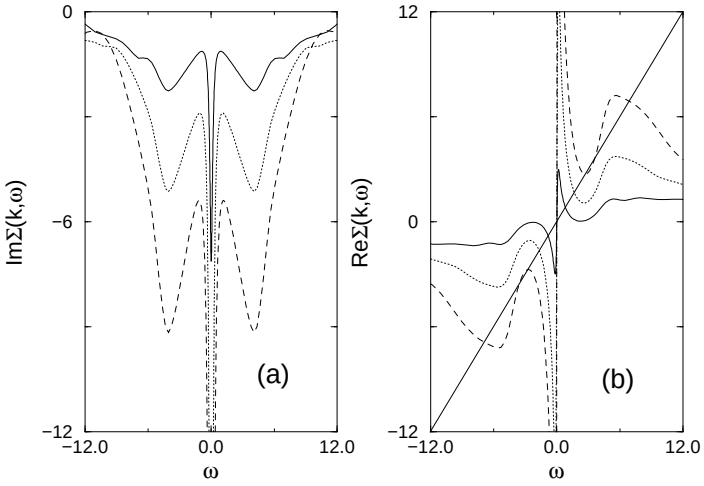

FIG. 4. (a) Imaginary and (b) real parts of the self-energy at $\vec{k} = (\pi/2, \pi/2)$ for U =4, 6 and 8 at $T = 0.1$ denoted as the solid, dotted and dashed curves, respectively. The solid straight line in (b) is $\omega - \varepsilon(\vec{k})$.

ferent bands. This feature is also similar to the one from the 1/d effect in the infinite dimensional Falicov-Kimball model [16]. The density of states obtained from the average of the spectral function in the whole Brillouin zone shows more suppressed antiferromagnetic bands and thus more pronounced Hubbard bands in Fig. 3(b) than the spectral function does at $(\pi/2, \pi/2)$.

As the interaction strength U is increased, the imaginary part of the self-energy grows rapidly both at the Fermi energy and in the intermediate frequency region ($\sim \pm 4$) shown in Fig. 4(a). The former comes from strong 2D critical fluctuations near half-filling and the latter mainly from the lowest order diagram (second order in U) which is responsible for the Hubbard bands for large enough U. As U is increased to 8 (dashed curve in Fig. 4(b)), seven solutions are found in the peak condition. The most outer two solutions lead to the Hubbard bands and the most inner two near the Fermi energy to the antiferromagnetic bands, and the other three accompanied by large scattering rates yield the incoherent background. This result is similar to the earlier report by Kampf and Schrieffer [13] of the developing multiple solutions in the peak condition by increasing the spin-spin correlation length. Besides the total number of solutions, however, there are some qualitative differences between these two results. Because of the insufficient treatment of the 2D critical fluctuations in their phenomenological antiferromagnetic spin fluctuation spectrum, their solution at the Fermi energy shows a single quasiparticle peak, while in our calculations a quasiparticle state is destroyed for a half-filled band. Due to the same reason, the pseudogap found in their paper does not come from a suppressed spectral weight inside the *antiferromagnetic* bands but instead inside the *Hubbard* bands.

In summary, we formulated a theory to the 2D Hubbard model in a manner free of finite size effect and numerical analytical continuation, yet containing the essential features of the 2D Hubbard model, i.e., the correct atomic limit for large ω and 2D spin fluctuations. As the temperature is decreased for a 2D half-filled band, anomalous behaviors are found near the Fermi energy such as a split peak in the spectral function, a large positive slope greater than unity in the real part of the self-energy and a strong local maximum in the scattering rates. As the interaction strength U is increased, four peaks associated with the antiferromagnetic and Hubbard bands begin to develop in the small and intermediate frequency regimes.

The author would like to thank Prof. P. Fulde for critical reading of the manuscript as well as for his valuable comments. Useful discussions with Drs. S. Blawid, R. Bulla, T. Dahm, P. Kornilovitch, M. Laad, W. Stephan, and numerous other colleagues in the Max Planck Institute for Physics of Complex Systems would like to be acknowledged.

[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[3] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[4] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[5] S. R. White, Phys. Rev. B **44**, 4670 (1991); M. Vekić and S. R. White, *ibid.* **47** 1160 (1993).
[6] C. E. Creffield *et al.*, Phys. Rev. Lett. **75**, 517 (1995).
[7] N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).
[8] N. E. Bickers and S. R. White, Phys. Rev. B **43**, 8044 (1991).
[9] T. Dahm and L. Tewordt, Phys. Rev. B **52**, 1297 (1995); J. J. Deisz, D. W. Hess, and J. W. Serene, Phys. Rev. Lett. **76**, 1312 (1996).
[10] Y. Vilk and A. M. Tremblay, to appear in J. Physics (Paris)(Nov.1997); cond-mat/9702188.
[11] N. F. Berk and J. R. Schrieffer, Phys. Rev. Lett. **17**, 433 (1966); P. C. E. Stamp, J. Phys. F: Met. Phys., **15**, 1829 (1985).
[12] Y. M. Vilk, Liang Chen, and A. M. Tremblay, Phys. Rev. B **49**, 13 267 (1994).
[13] A. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990); *ibid.* **42** 7967 (1990).
[14] A. Moreo *et al.*, Phys. Rev. B **51**, 12 045 (1995).
[15] R. Preuss, W. Hanke, and W. von der Linden, Phys. Rev. Lett. **75**, 1344 (1995).
[16] M. Laad and M. Van den Bossche (unpublished).